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Two-loop self-energy contribution to the Lamb shift in H-like ions

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The two-loop self-energy correction is evaluated to all orders in $Z\alpha$ for the ground-state Lamb shift of H-like ions with $Z \geq 10$, where Z is the nuclear charge number and α is the fine structure constant. The results obtained are compared with the analytical values for the $Z\alpha$-expansion coefficients. An extrapolation of the all-order numerical results to $Z = 1$ is presented and implications of our calculation for the hydrogen Lamb shift are discussed.

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Hydrogen and hydrogen-like ions are the simplest atomic systems, whose studies inspired the creation and development of modern quantum electrodynamics (QED). Despite their apparent simplicity, two-body atomic systems continue to challenge physicists after more than a century of research. On the experimental side, the absolute frequency of the $1s$-$2s$ transition in atomic hydrogen has lately been measured to 1.8 parts in 10^{14} [1], which represents an improvement of accuracy by 4 orders of magnitude achieved during the last twenty years. On the theoretical side, the largest error for the $1s$-$2s$ transition energy stems presently from the uncertainty in the experimental value for the proton charge radius [2], even with the most recent reanalysis of electron-proton scattering data [3]. Apart from that, the major theoretical uncertainty comes from the two-loop QED effects. Important progress achieved recently in investigations of two-loop corrections to order $\alpha^2(Z\alpha)^6$ [4, 5] resulted in a much better theoretical understanding of the hydrogen Lamb shift. Consequently, in the latest adjustment of fundamental constants [6], the value for the proton charge radius (which enters as a parameter into the determination of the Rydberg constant) was obtained by comparing spectroscopic data for the $1s$-$2s$ transition in hydrogen with the corresponding theoretical prediction.

The results of refs. [4, 5] were obtained within the traditional approach based on a semi-analytic expansion of binding QED corrections in $Z\alpha$ and $\ln[(Z\alpha)^{-2}]$ (Z is the nuclear charge number and α is the fine structure constant). A peculiar feature of the two-loop effects (first of all, the two-loop self-energy correction) is that this expansion converges very slowly even in case of hydrogen. Numerical values of the expansion coefficients are large and tend to grow with increase of the order, which makes estimations of uncertainties due to higher-order effects rather problematic. Moreover, complexity of calculations of the $Z\alpha$-expansion coefficients grows drastically with the increase of their order, so that the derivation of the complete contribution to the next order $\alpha^2(Z\alpha)^7$ does not seem feasible in the near future.

An alternative approach is to perform the investigation non-perturbatively in the parameter $Z\alpha$. For one-loop corrections, such calculations extended over three decades [7, 8, 9, 10]. A non-perturbative evaluation of two-loop QED effects is a much more demanding problem. The dominant contribution (especially in the low-Z region) stems from the two-loop self-energy correction, which is considered to be the most problematic two-loop QED effect. A calculation of this correction to all orders in $Z\alpha$ was started in refs. [11, 12] and completed in a series of our investigations [13, 14, 15]. Up to now, the calculation of the two-loop self-energy correction was carried out for ions with $Z \geq 40$ only. Large numerical cancellations growing fast when Z was decreased prevented us from calculating this correction for lower-Z ions and from drawing any definite conclusions about agreement of our results with the known $Z\alpha$-expansion terms. The goal of the present investigation is to perform a calculation of the two-loop self-energy correction for ions with $Z \geq 10$ and to compare our non-perturbative treatment with the previous investigations within the $Z\alpha$-expansion approach.

We start with summarizing the results available for the $Z\alpha$ expansion of this correction for the ground state of H-like ions. The corresponding energy shift is conveniently represented in terms of a dimensionless function

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$F(Z\alpha)$ (relativistic units $\hbar = c = 1$ are used throughout the paper),

$$\Delta E = m \left(\frac{\alpha}{\pi}\right)^2 \frac{(Z\alpha)^4}{n^3} F(Z\alpha)\,, \tag{1}$$

where n is the principal quantum number and the $Z\alpha$ expansion of the function F reads

$$F(Z\alpha) = B_{40} + (Z\alpha)B_{50} + (Z\alpha)^2\Big[L^3 B_{63} + L^2 B_{62} + L\,B_{61} + G_{\rm h.o.}(Z\alpha)\Big]\,, \tag{2}$$

where $L = \ln[(Z\alpha)^{-2}]$ and $G_{\rm h.o.}$ is the higher-order remainder whose expansion starts with a constant, $G_{\rm h.o.}(Z\alpha) = B_{60} + Z\alpha\,(\dots)$. The results presently available for the expansion coefficients (see refs. [2, 4, 5] and references therein) are:

$$B_{40}(ns) = 1.409\,244\dots\,, \tag{3}$$
$$B_{50}(ns) = -24.2668(31)\,, \tag{4}$$
$$B_{63}(ns) = -8/27\,, \tag{5}$$
$$B_{62}(1s) = 16/27 - (16/9)\ln 2\,, \tag{6}$$
$$B_{61}(1s) = 49.838317\,, \tag{7}$$
$$B_{60}(1s) = -61.6(9.2)\,. \tag{8}$$

Contrary to the calculations summarized above, our present consideration does not rely on the $Z\alpha$ expansion. The working frame is the Furry picture, where the interaction of the electron with the nucleus is taken into account to all orders right from the beginning. The price to pay is that we have to deal with the *bound*-electron propagators, whose structure is much more elaborate than that of the *free*-electron propagator. The detailed analysis of the two-loop self-energy correction was presented in our previous investigation [15] and will not be repeated here. In this Letter we just mention the major problems to be tackled in order to obtain reliable numerical results in the low-Z region and sketch the ways of their solutions. (To note, numerical cancellations for the lowest value of Z considered here, $Z = 10$, amount to 4 orders of magnitude.)

One of the main factors that influences the numerical accuracy of the final result is its dependence on the size of the basis set used in the evaluation of the P term (see ref. [15] for details). In the present work, a new *dual-kinetic-balance* [16] basis set was employed, which considerably improved the convergence in the low-Z region. In addition, the actual calculation was repeated several times with increasing numbers of basis functions N and then an extrapolation $N \to \infty$ was performed. We note, however, that despite the improvement achieved, the dependence of the P term on the basis set is still one of the major sources of the uncertainty. Another difficulty in the evaluation of the P term was to properly control the accuracy of numerical integrations over momentum variables. It is associated with a significant contribution coming from the region of very large momenta, where the numerical Green function is not smooth enough, due to restrictions of a finite-basis-set representation. The problem has been handled by introducing a set of subtractions that have the same behavior for large momenta as the original integrand but are easier to evaluate numerically, and by employing very fine grids for numerical momentum integrations. The calculation of the M term (see ref. [15] for details) was carried out employing the contour C_{LH} for the integrations over the virtual-photon energies, which is much more suitable for the numerical evaluation in the low-Z region than the integration simply along the imaginary axis. In addition, a contribution containing the dominant part of the spurious behavior in the low-Z region was separated from the M term and calculated separately. It involves only one infinite partial-wave expansion, which makes its numerical computation easier as compared to the full M term.

In the table, we present the numerical results obtained for the two-loop self-energy correction for the ground state of H-like ions with $Z \geq 10$. As compared to our previous investigations [14, 15], new calculations for $Z = 10$ – 30 were performed and the numerical accuracy for $Z = 40$, 50, and 60 was improved. The numerical values for $Z \geq 70$ are taken from our previous investigation [15]. In fig. 1, our non-perturbative (in $Z\alpha$) results are compared with the contribution of the known coefficients of the $Z\alpha$ expansion, as given by eqs. (3)-(8). We observe that the numerical results behave smoothly and tend to approach the known analytical value at $Z = 0$.

In order to perform a more detailed comparison with the $Z\alpha$-expansion calculations, we separate the higher-order remainder $G^{\rm h.o.}(Z\alpha)$ [defined by eq. (2)] from our non-perturbative results, with the corresponding plot presented in fig. 2. As can be seen from the figure, a naively estimated limit of our numerical values at $Z = 0$ is about twice as large as the analytical result (8) for the coefficient B_{60}. However, there is an indication [17] that the analytical result of ref. [4] for the coefficient B_{61} is incomplete. In this case, the numerical data for $G^{\rm h.o.}$ plotted in fig. 2 contain an admixture of the logarithmic contribution to the leading order and, therefore, are not bound at $Z = 0$. Until analytical calculations of B_{61} have been finished, we cannot draw any conclusions concerning agreement with the existing result for B_{60}.

It is possible, however, to extrapolate our numerical results for $G^{\rm h.o.}(Z\alpha)$ to $Z = 1$ and to obtain an approx-

imate value for the corresponding higher-order contribution for the hydrogen Lamb shift. For such extrapolation, we use the procedure first employed in ref. [18] and recently described in detail in ref. [19]. The approximate value for $G^{\rm h.o.}(1\alpha)$ is obtained in two steps. First we apply an (exact) linear fit to each pair of two consecutive points from our data set and store the resulting value at $Z = 1$ as a function of the average abscissa of the two points of the original set. (The points with $Z = 10$ and 15 are not employed for the extrapolation because of their large error bars.) Then, we perform a global linear or quadratic least-squares fit to the set of data obtained and take the fitted value at $Z = 1$ as a final result.

In order to test this extrapolation scheme and to check the consistency of our numerical data with the first $Z\alpha$-expansion coefficients, we consider the function

$$\widetilde{F}(Z\alpha) = \frac{F(Z\alpha) - B_{40}}{Z\alpha} = B_{50} + (Z\alpha)(\cdots)\,. \qquad (9)$$

The extrapolation procedure described above yields a result that reproduces the analytical value for the B_{50} coefficient within the 15% accuracy. Applying the same extrapolation scheme to the higher-order remainder, we obtain

$$G^{\rm h.o.}(1\alpha) = -127 \pm 30\%\,. \qquad (10)$$

The error bars indicated are obtained by applying the extrapolation procedure to the function $G^{\rm h.o.}(Z\alpha) + 10\,\ln(Z\alpha)^{-2}$, which is supposed to account for the probable incompleteness of the present result for the B_{61} coefficient.

The result (10) significantly alters the previous prediction for the higher-order remainder [5], which reads (in our notations)

$$G^{\rm h.o.}(1\alpha;{\rm old}) = -61.6 \pm 15\%\,. \qquad (11)$$

The difference between (10) and (11) leads to a shift of the latest prediction for the hydrogen $1s$ Lamb shift [5] by 7 kHz, with the result

$$\nu(1s) = 8\,172\,804\,(32)(4)\,{\rm kHz}\,, \qquad (12)$$

where the first error stems from the current uncertainty of the proton charge radius and the second one is the theoretical uncertainty corresponding to the one of eq. (10). We note that significant progress in the determination of the proton radius is anticipated in the near future from the experiment on the muonic hydrogen, which is currently being pursued in Paul Scherrer Institute [20].

To sum up, we have performed a non-perturbative (in $Z\alpha$) calculation of the two-loop self-energy correction that extends our previous evaluation to the region $Z \geq 10$. The numerical results obtained agree well with the first two terms of the $Z\alpha$ expansion. A certain disagreement is found with the analytical results to order $\alpha^2(Z\alpha)^6$, which could possibly be associated with incompleteness of the present value for the B_{61} coefficient. An extrapolation of the numerical data to $Z = 1$ yields a result that alters the theoretical value for the the hydrogen $1s$ Lamb shift by 7 kHz.

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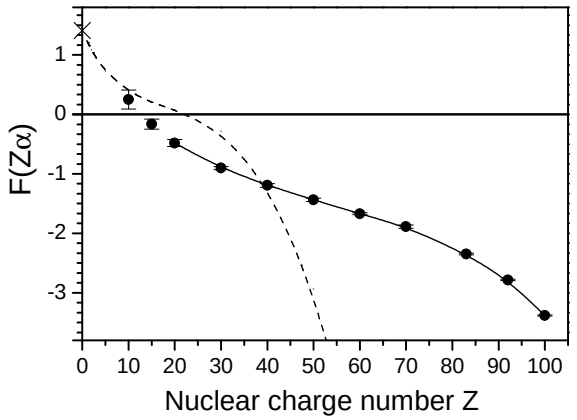
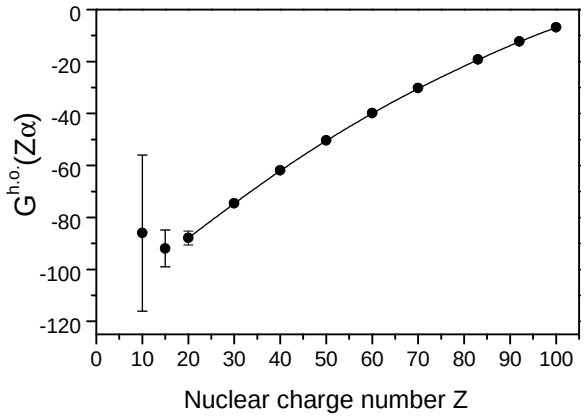


The two-loop self-energy correction evaluated to all orders in $Z\alpha$ (dots) together with the contribution of all known terms of the $Z\alpha$ expansion (dashed line), in terms of $F(Z\alpha)$. The cross indicates the analytical value of this correction at $Z = 0$.



Higher-order remainder $G^{\mathrm{h.o.}}(Z\alpha)$ defined by eq. (2).

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Individual contributions to the two-loop self-energy correction expressed in terms of $F(Z\alpha)$.

Z	LAL	F term	P term	M term	Total
10	−0.3577	822.14(2)	−721.34(12)	−100.19(10)	0.25(16)
15	−0.4951	292.902(13)	−235.205(70)	−57.366(48)	−0.164(85)
20	−0.6015	136.911(7)	−102.026(55)	−34.764(16)	−0.481(58)
30	−0.7565	44.729(3)	−29.410(25)	−15.465(5)	−0.903(26)
40	−0.8711	19.505(3)	−11.575(30)	−8.253(5)	−1.194(31)
			−11.41(15)[a]	−8.27(18)[a]	−1.05(23)[a]
50	−0.9734	10.025(2)	−5.488(26)	−5.001(3)	−1.437(26)
			−5.41(8)[a]	−4.99(6)[a]	−1.34(10)[a]
60	−1.082	5.723(1)	−2.970(18)	−3.341(2)	−1.670(18)
			−2.93(4)[a]	−3.342(21)[a]	−1.63(4)[a]
70	−1.216	3.497(1)	−1.757(25)	−2.412(11)	−1.888(27)
83	−1.466	1.938	−1.057(13)	−1.764(4)	−2.349(14)
92	−1.734	1.276	−0.812(10)	−1.513(3)	−2.783(10)
100	−2.099	0.825	−0.723(7)	−1.384(3)	−3.381(8)

[a] ref. [15].